ISSN: 3068-0352

Katalyst Publishers

Open Access

Journal of Current Trends in Physics Research and Applications

Short Commentary

Aquasiclassical Trajectory Study of The Reaction of Chlorine Atom with Silane Based on a Novel Particle Swarm Optimization Algorithm

Ang-Yang Yu[1*]; Huan Yang[2] and Yu-Jun Zheng[2]

[1]Xiamen University of Technology;No.600 Ligong Road, Jimei District, Xiamen, 361024, Fujian Province, China

[2]School of Physics; Shandong University, Jinan, 250100, China

***Corresponding Author:**

Dr. Angyang Yu, Xiamen University of Technology;No.600 Ligong Road, Jimei District,Xiamen, 361024, Fujian Province, China;
E-Mail: wisdomyay@ustc.edu

Received Date: 29th Nov, 2025
Accepted Date: 01st Dec, 2025
Published Date: 03th Dec, 2025

Abstract

Quasi-Classical Trajectory(QCT) method is a famous approach in the realm of molecular reaction dynamics. Generally, the integration of Hamiltonian equations in QCT employs the fourth-order Runge-Kutta method. Occasionally, symplectic algorithm is adopted in order to achieve better conservation of the total energy and the total angular momentum of a specific reaction system. In this work, a novel particle swarm optimization(PSO) algorithm has been put forward in order to improve the availability of the integration of Hamiltonian equations. Based on this new scheme, calculations of the total reaction cross section, the microscopic rate constant, and the thermal rate constant have been performed for both the reaction of chlorine atom with silane. This work can not only help evaluate the PES adopted, but also examine the performance of the new PSO algorithm for QCT. We believe that the proposed PSO algorithm is an effective numerical integral scheme, which can help promote the development of molecular reaction dynamics.

Citation: **Dr. Angyang Yu** (2025) Aquasiclassical trajectory study of the reaction of chlorine atom with silane based on a novel particle swarm optimization algorithm. J Cur Tre Phy Res App 3(9): 1-1.